

Chu Xin (Cloris) Cheng

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EDUCATION

California Institute of Technology

B.S. Computer Science

Pasadena, CA

Sep. 2021 – Jun. 2025

- **Cumulative GPA:** 4.3
- **Relevant Coursework:** Introductory Methods of Computational Mathematics, Data Mining and Machine Learning, Statistical Inference, Fundamentals of Statistical Learning, Advanced Topics in Machine Learning, Applied Linear Algebra, Applied Real and Functional Analysis, Game Theory, Stochastic Processes and Regression, Mathematical Optimization.

LIST OF PUBLICATIONS

Atomic Diffusion Models for Small Molecule Structure Elucidation from NMR Spectra

Ziyu Xiong, Yichi Zhang, Foyez Alaaddin, Chu Xin Cheng, Joon Soo An, Mohammad R. Seyedsayamdost, Ellen D. Zhong

Neural Information Processing Systems (NeurIPS), 2025.

Available: <https://openreview.net/pdf?id=STsjfx2cee>

How to Unlock Time Series Editing? Diffusion-Driven Approach with Multi-Grained Control

Hao Yu*, Chu Xin Cheng*, Runlong Yu, Yuyang Ye, Shiwei Tong, Zhaofeng Liu, Defu Lian

arXiv preprint, 2025.

Available: <https://arxiv.org/pdf/2506.05276>

Preferential Bayesian Optimization with Multiple Mixed Objectives

Raul Astudillo, Kejun Li, Maegan Tucker, Chu Xin Cheng, Aaron Ames, Yisong Yue

Transactions on Machine Learning Research (TMLR), 2025.

Available: <https://openreview.net/pdf?id=mjsoESaWDH>

Practical Bayesian Algorithm Execution via Posterior Sampling

Chu Xin Cheng*, Raul Astudillo*, Thomas Desautels, Yisong Yue

Neural Information Processing Systems (NeurIPS), 2024.

Available: <https://arxiv.org/pdf/2410.20596>

Improving sample efficiency of high dimensional Bayesian optimization with MCMC

Zeji Yi*, Yunyue Wei*, Chu Xin Cheng*, Kaibo He, Yanan Sui

Learning for Dynamics & Control Conference (L4DC), 2024.

Available: <https://proceedings.mlr.press/v242/yi24a/yi24a.pdf>

HONORS AND AWARDS

Hertz Fellow

2025

Fannie and John Hertz Foundation

- The Hertz Fellowship is awarded annually to the nation's most promising graduate students in applied physical and biological sciences, mathematics, and engineering. Fellows receive five years of funding and commit to applying their work to address critical challenges facing society.

Bhansali Family Prize in Computer Science

2025

California Institute of Technology

- Established in 2001 by Vineer Bhansali (B.S. '87, M.S. '87) in memory of his grandfather, Mag Raj Bhansali. The prize and honorarium are awarded to an undergraduate student for outstanding research in computer science in the current academic year. Recipients are selected by a committee of computer science faculty.

Finalist, Undergraduate Operations Research Prize

2024

Institute for Operations Research and the Management Sciences

- The Undergraduate Operations Research Prize Competition is held each year to honor students who conducted original and significant theoretical and/or applied research in the field of operations research or management science during their undergraduate enrollments. All finalists of the competition are invited to present their research at the INFORMS Annual Meeting.

Jack E. Froehlich Memorial Award

2024

California Institute of Technology

- The award is presented to a junior in the upper 5 percent of their class who shows outstanding promise for a creative professional career.

Henry Ford II Scholar Award

2024

California Institute of Technology

- The award is presented annually to engineering students with the best academic record at the end of the third year of undergraduate study.

WORK AND RESEARCH EXPERIENCES

Machine Learning Researcher, Gridmatic

Spring 2025

Cupertino, CA

- Research on generative modeling for time series forecasts; in particular, enhanced day-ahead electricity-price forecasting by incorporating super-resolution features into a generative time series model. Curated datasets and built models for predicting congestion in power grids.

Machine Learning Researcher, Yisong Yue's Group

2022 - 2024

California Institute of Technology / Lawrence Livermore National Lab

Project 1, 2022 Generalized traditional Bayesian optimization methods to learn from preference feedback within the dueling bandits framework, with an extension to continuous space utilizing Gaussian processes. Developed an algorithm that incorporates Langevin dynamics and Kalman filtering on the posterior distribution to leverage gradient feedback.

Project 2, 2023 Contributed to developing the first theoretical framework for multi-attributed preferential Bayesian optimization, aimed at its application to exoskeleton gait optimization. Designed an algorithm that employs Chebyshev scalarization to produce Pareto-optimal actions.

Project 3, 2023 Investigated machine learning methods for protein engineering, focusing on antibody design. Applied feature conformal prediction to Graph Neural Networks to obtain confidence intervals with guaranteed coverage for modeling the fitness function with uncertainty.

Project 4, 2024 Developed a new Bayesian computation algorithm, PSBAX, to infer properties of unknown functions by selecting points based on posterior probability. Demonstrated its superior performance across multiple domains, including real-world protein engineering datasets. Contributed to a rigorous analysis of its convergence guarantees, advancing the theoretical foundations of posterior sampling. Currently collaborating with Lawrence Livermore National Lab to apply PSBAX to antibody portfolio optimization.

Machine Learning Researcher, Zhong Lab

2024

Princeton University

Summer Undergraduate Research Fellowship

- Research on investigating machine learning models for accelerating small molecule discovery by predicting chemical structures from NMR data with Prof. Ellen Zhong. Achieved 98.9% accuracy using a multilabel classifier to identify amino acid groups in peptides from synthetic NMR spectra. Ongoing work focuses on refining model architectures and expanding datasets for full sequence prediction. The work aims to eventually automate structure elucidation from new natural products, which has profound impact in drug development and chemical biology.

Machine Learning Researcher, Rigorous Systems Research Group

2022 - 2023

California Institute of Technology

- Research with Prof. Adam Wierman focused on optimization and control, particularly in the realm of online policy selection. Investigated the generalization of optimization algorithms to nonlinear dynamical systems with non-convex reward functions.

Research Assistant

2022

California Institute of Technology / Tsinghua University

Summer Undergraduate Research Fellowship

- Research with Prof. Yanan Sui on high-dimensional sampling using Bayesian optimization with Gaussian processes, specifically focused on its application in spinal stimulation. Employed Markov chain Monte Carlo techniques and Langevin dynamics to efficiently sample from intractable posteriors and devised an algorithm capable of maintaining an adaptive mesh on a high-dimensional action space.

Intern, Tencent (Tencent Xinghuo Program)

2021 - 2022

Shenzhen, Tencent Quantum Lab

- Reproduced quantum approximate optimization algorithm using Tensorflow and Qiskit. Studied quantum information and quantum computation with focus on algorithms such as Grover search and variational algorithms.

TEACHING EXPERIENCES

Teaching Assistant

2022 - 2024

California Institute of Technology

- Responsible for leading recitations, holding weekly office hours, and writing up and grading problem sets. The average class size is 100 students.
- Courses: Data Mining and Machine Learning (2023 Winter & 2024 Winter), Statistical Inference (2023 Spring & 2024 Spring), Applied Linear Algebra (2024 Fall), Introduction to Probability Models (2023 Fall).

EXTRACURRICULAR EXPERIENCES

Competitions Expert, Kaggle

2021 - 2022

Online

- Sartorius - Cell Instance Segmentation: Top 4%, Rank 46/1505. Computer vision contest for object detection. Used popular frameworks such as Mask R-CNN and libraries such as MMDetection and Detectron2.
- Feedback Prize - Evaluating Student Writing: Top 8%, Rank 159/2058. NLP contest for text segmentation and classification. Used models such as Transformer, BERT, ELMo.

TECHNICAL SKILLS

Languages: Python, C, Java, OCaml, Swift, MATLAB.

ML Packages: PyTorch, TensorFlow, Pandas, SciPy.